Ethyl 1-thio-beta-D-galactopyranoside

56245-60-4 | DTXSID70440378

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 139 °C

Global applicability domain: Inside

Local applicability domain index: 4.46e-01

Confidence level: 6.37e-01

Nearest Neighbors from the Training Set

Image not found

Isopropyl beta-D-1-
thiogalactopyranoside
Measured: 121
Predicted: 132

Image not found

Methyl alpha-D-glucopyranoside
Measured: 168
Predicted: 163